THE WORLD OF CHEMISTRY

Program #4

MODELING THE UNSEEN

Producer Doug Bolin

Air Script: October 31, 1988

PRODUCED BY

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Annenberg/CPB Project Logo and Music

Funder Credits

MONTAGE: Computer graphics, chemists at work, drugs, volcanos

NARRATOR (MUSIC and NAT SOUND under):
A riddle. If chemistry is a science in search of facts, why is imagination so important? The answer is wrapped in mysteries. Why are there enormous volcanos of liquid sulfur on this distant planet? How do drugs work inside our bodies? And what explains the behavior of gases at different pressures? Chemists must probe events which cannot be observed directly. So imagination is the first step towards modeling the unseen.

SUPER: MODELING THE UNSEEN

THE WORLD OF CHEMISTRY OPEN: Montage, Music, Logo

RH in art gallery

ROALD HOFFMANN (SYNC):
I'm in one of my absolutely favorite places, the East Wing of the National Gallery in Washington. Let's take a look at some sculptures. Here is this marvelous sculpture by Alberto Giacometti, a seated woman, less elongated than his usual representations. You know, no doubt Giacometti used a clay model in constructing this bronze figure, and, in another sense of the word "model," this sculpture, all art, gives us a representation of the essence of some expression of an emotion of some response to a piece of the natural world around. The artist is trying to understand that world. Chemists also want to understand the world that we live in, and in order to do that, we have to form hypotheses and models. The models that we use are different from those that artists have -- for instance, different from this beautiful sculpture by Isamu Noguchi. Chemists are often trying to observe things that we cannot see or touch directly.

MONTAGE: Gases, coal on conveyor belt, computer graphics and models, chemists at work in lab, microscope shots, volcanos

NARRATOR (MUSIC and NAT SOUND under):
Some things are too complex to study directly. A gas consists of billions of tiny particles. There are too many of them to observe all at once. So models are used to predict their behavior. Some processes happen too slowly. The geochemical events that produced this coal took place over millions of years. Some things are too far away to study firsthand. The chemistry on these outer planets can only be guessed through long range and indirect observations. Even when we can observe events close up, we may still need models to understand the chemistry that produced them. From the chemistry of the largest bodies in our universe to the behavior of particles so small they are invisible, chemists use models to imagine, then test explanations. They need models because these events are like black boxes that can't be opened. How do scientists make models to reveal such inner mysteries? To unlock these secrets, series demonstrator Don Showalter went to a class of sixth graders.

DS in classroom
with students

DON SHOWALTER (SYNC):
We're here to solve a problem for you today. Many times in chemistry, what we are studying we really can't see very well. In fact, we might not be able to see at all. So what we want to do, a little bit of an experiment with you today, and the experiment involves these two boxes. What we want to do is find out what's inside these boxes. All right. The box is locked so that we can't see inside the box. Now, what we want you to do is form in your mind a model. Do you know what a model is?

STUDENTS (SYNC):
Yes.

DON SHOWALTER (SYNC):
What is a model? A model, sort of the idea -- not a model like a model airplane, but maybe a model of a mental picture, huh? What could you do to be able to tell what's inside the box? How about if I pass it around. And now, what I want you to do is to form a mental picture in your mind of what's inside that box? What do you notice about the two boxes, in comparison? All right. One's heavy, one is light. All right. What else? What about --

CHILD (VO):
One makes sound and one doesn't.

DON SHOWALTER (SYNC):
Good. Say it real loud.

CHILD (VO):
One makes sound and one doesn't.

DON SHOWALTER (SYNC):
You betcha. One makes sound and one doesn't. Have you got a mental picture yet? What's inside? What's inside the light one?

CHILD (SYNC):
I don't know. It's either big or else there's nothing in there.

DON SHOWALTER (SYNC):
Anyone else?

CHILD (SYNC):
I think there's nothing because, when you shake it, you don't hear anything. And it's light.

DON SHOWALTER (VO):
So using your ears, huh?

CHILD (SYNC):
I think that there's like sponge or something soft in the box, because when you shake it, you don't hear anything, but the box feels heavier than if it were empty.

DON SHOWALTER (SYNC):
Okay. All right. Now, I want you to hold on to that idea for a minute. All right. Now we want to hear about the heavy box over here, hear the heavy people over here, huh? All right now.

CHILD (SYNC):
I think there's change in the box because when you shake it, you hear like chains going against the box, and it's heavy.

DON SHOWALTER (SYNC):
You hear what kind of a sound?

CHILD (VO):
Clanking.

DON SHOWALTER (SYNC):
Like a rattling or a clank, clanking sort of a sound in there, huh? And what else about the box.

CHILD (VO):
It's real heavy.

DON SHOWALTER (SYNC):
It's heavy. It's heavy, so there's something in there that is dense. Do you know what that word means, dense? Okay. Anyone else wanna give us an idea about the heavy box?

CHILD (SYNC):
I think there's just any kind of metal in there, because the noise it makes.

DON SHOWALTER (SYNC):
Any way we could look inside things without actually opening them up?

CHILD (SYNC):
We could X-ray the box to check what's in there.

DON SHOWALTER (VO):
All right. We've done that. Do you want to see them?

CHILD (VO):
The heavy one.

DON SHOWALTER (SYNC):
That's the heavy one. What do you see in there?

STUDENTS (VO):
Nuts, bolts, screws.

DON SHOWALTER (SYNC):
All right. Boy, we were close, weren't we? You were right on. You were thinking that it had all that metal in there, and certainly the X-ray shows it up. So we could study that box without even opening it up. Okay. What do you see in here?

STUDENTS (VO):
Nothing.

DON SHOWALTER (SYNC):
All right. So we say nothing in that box, huh?

CHILD (SYNC):
Right.

DON SHOWALTER (VO):
Everybody agree?

STUDENTS (SYNC):
Yes.

DON SHOWALTER (VO):
All right. Everybody in agreement, hold their hand up? All right. Let's open these boxes up and see what's inside there, huh? All right. Now, this one. Do you feel confident that this has nuts and bolts in it?

STUDENTS (VO):
Yes.

DON SHOWALTER (SYNC):
You're right on. You're right on. Look what's inside that box.

CHILD (VO):
Nuts and bolts.

DON SHOWALTER (SYNC):
Nuts and bolts, huh? All rightee. How about this box? What do we say?

STUDENTS (VO):
Nothing.

DON SHOWALTER (SYNC):
Nothing inside there.

CHILD (VO):
Possibility.

DON SHOWALTER (SYNC):
Possibility of having nothing inside. Here we go. All right.

STUDENTS (SYNC):
Cotton balls!

DON SHOWALTER (VO):
Cotton balls.

(NAT SOUND: Clapping)

MONTAGE: Freeze frames of students and DS

NARRATOR (MUSIC under):
The steps a scientist follows to develop a model are along the same path traced by the students. First, scientists make general observations about a situation and closely observe the behavior of the system being studied. (cont.)

NARRATOR cont:Then, relating these observations to their past experience, scientists try to imagine what model could explain their observations. Like the students, they build the model based on their past experience and their ongoing observation. Next, scientists must test their models. The students tested their models by examining X-rays of the two boxes. These tests are designed to confirm or disprove the model. One procedure, the X-ray test, supported a model that was false. When the box that looked empty was opened, it contained cotton balls. So scientists test their models using many different procedures. How does this method work in the real world? Let's start with a model of something on a very large scale.

Computer graphics of space and the solar system, observatory, telescope

NARRATOR (MUSIC under):
For centuries, scientists have been studying this kind of black box, our solar system. Until recently, these observations were limited to what could be seen through telescopes. We have had to rely heavily on models to explain the chemistry of these enormous bodies. One of these models concerned Io, the first moon of Jupiter. (cont.)

NARRATOR cont:
Dr. Torrence Johnson is director of the Voyager Project.

INTERVIEW: Dr. Torrence Johnson, Director, Voyager Project, JPL

SUPER: Torrence Johnson

DR. TORRENCE JOHNSON (SYNC):
Before we got the spacecraft out to the Jovian system, basically what we knew about Io was how big it was, how much it weighed, and how bright it was, to first order. How big it was and how much it weighed made it look just like the Earth's moon. So you started all of our modeling assumptions in the early days, before Voyager started, with the idea that Io was gonna be basically like the moon. There was one problem. It was about ten times brighter than the moon, in terms of its surface reflectance.

View of Earth from space, volcanos, lava flow

NARRATOR (MUSIC and NAT SOUND under):
Why was Io so bright? One model proposed that, unlike our moon, Io had once been covered with great amounts of water, volcanic activity had caused the water to evaporate, leaving behind a bright layer of salt deposits.

INTERVIEW: Dr. Torrence Johnson cont.

DR. TORRENCE JOHNSON (SYNC):
But, because it was the same size as the moon, we thought that all of this heating activity had occurred three to four billion years in the past, just as the moons had. So we thought it was dead. Our model was of a dead lunar interior with a salty outside probably blasted full of craters by meteorites.

Rocket launch, animated graphics of satellite

NARRATOR (MUSIC and NAT SOUND under):
In 1977, the first Voyager probe was launched to gather observations on Jupiter and Io from close range. Scientists waited for 18 months as Voyager made its lonely pilgrimage. The wait was worth it.

INTERVIEW: Dr. Torrence Johnson cont.

DR. TORRENCE JOHNSON (SYNC/VO):
What Voyager found, of course, was fantastically exciting. It found a body that's more volcanically active than any object we've ever seen in the solar system. (cont.)

Slides of Io

DR. TORRENCE JOHNSON cont:
The surface is covered with huge volcanic features, large collapse pits, calderas, volcanic flows, and most exciting of all, we caught several active volcanic eruptions in the process of going on, with Voyager I, throwing plumes of debris up a hundred to three hundred kilometers above the surface.

Computer graphics of Io, volcanos, geysers

NARRATOR (MUSIC and NAT SOUND under):
What could be the source of the energy for these volcanos? Investigators propose the following model: Io hangs in space between Jupiter at one end and Europa at the other. The gravitational force from each body tugs on Io, causing it to flex and heat up, as represented here in exaggerated form. So, in this model, gravitational energy generates the heat for the volcanism. But there was still something strange about the chemistry of these volcanos. They weren't volcanic eruptions like the ones here on Earth, with lava exploding or flowing out of the ground. Instead, they resulted from the same conditions that produced geysers, such as the ones in Yellowstone Park.

INTERVIEW: Dr. Torrence Johnson cont.

DR. TORRENCE JOHNSON (SYNC): But they weren't water. We knew there wasn't any water now on Io, with respect to a spectroscopic evidence of that, so they proposed that the working fluid in this model was liquid sulfur or liquid sulfur dioxide, which can exist in liquid state fairly -- at fairly shallow depths below Io's crust.

GRAPHIC: Io differentiation

NARRATOR (MUSIC under): But this raised another enigma. How did sulfur compounds instead of silicate rocks come to be the dominant lava on Io's surface? A new model arose. It proposed that, long ago, silicate rock sank to the interior of Io. Water evaporated from the surface. Sulfur compounds were the lightest materials not to boil away. They ended up as the dominant lava. Is this the final model of Io's sulfur plumes?

INTERVIEW: Dr. Torrence Johnson cont.

DR. TORRENCE JOHNSON (SYNC): Well, when you build a model like this, you shouldn't get to thinking that the model represents reality. It will always change. In fact, we're not doing our job right if it doesn't change. It will always evolve as we get more information and revise our methods of observation based on the models.

RH in observatory

ROALD HOFFMANN (SYNC):
The chemical processes on Io are vast in scale, and Io is very far away. A lot of chemistry involves an intellectual excursion in another direction, to the very small. Take, for instance, a gas. We can measure its volume, its temperature, its pressure. But what is really happening inside a gas?

Chemists working in lab

NARRATOR (MUSIC under):
In order to understand, predict, and control what is happening inside a gas, we use a model called the kinetic particle model of gases. It assumes that a gas consists of large numbers of extremely small particles. There are billions of these particles in one breath of air. Let's make some observations and see how this model explains them.

DS in lab

DON SHOWALTER (SYNC):
This apparatus that we have here will allow us to measure the pressure of a gas. Now, what we want to study now in our model here is several different variables: pressure, volume, and the amount of gas. One thing we're not going to vary is the temperature. We're gonna hold that constant. The temperature of the room now remains the same. (cont.)

DON SHOWALTER cont:
Okay. Let's do an experiment. What I want to do is add an amount of gas to this already trapped volume of gas in here. As I do, of course, you know that's going to increase the pressure. Right? I'm gonna add some helium. Look at the pressure. I'm doubling the pressure. Once it's up there, I'll shut that off. Now, what I have done is double the pressure of the gas. Now, what do you think that means in terms of the amount of gas added? I bet you said it doubled the amount of gas, huh? That's the intuitive guess. And you're right. If we double the amount of gas, we double the pressure. Now, we want our model to be able to explain that.

GRAPHIC: Gas particles and pressure

NARRATOR (MUSIC under):
This is a representation of the container we used in our experiment with a vast number of gas particles already in it. The particles are moving chaotically in all directions and colliding with the walls of the container. For the purposes of our model, suppose that we could make the gas particles enormously larger and see them in slow motion. And to make things even clearer, we'll focus in on the behavior of just a few particles. (cont.)

NARRATOR cont:
As these particles collide with the walls of the container, the many tiny collisions exert a force on the walls. The force exerted on each unit of area of wall is the pressure of the gas, shown here on this gauge. What would happen if we doubled the number of the particles in the container? There are now twice as many collisions per second against the wall. What does this do to the pressure of the gas? It will double it, because the number of collisions in a given unit area is directly related to the pressure of the gas. The more collisions in a given unit of area, the higher the pressure.

DS in lab

DON SHOWALTER (SYNC):
Let's do a second experiment now. This time we're going to vary the volume and the pressure, again leaving temperature constant. Now what I'm gonna do is release the piston and see if it can come up to this mark here which refers to double of the volume. As we release the piston, it comes up to double the volume, and look what happened to the pressure. The pressure now is half of what it was. It was on 2, and now it's back down to just a little bit below 1. It's down to about what it was originally. So we have doubled the volume and, in the process, the pressure was cut in half. (cont.)

DON SHOWALTER cont:
That's another observation that we've had. So we've done two experiments now involving the amount of gas and the pressure. In the second experiment now, we looked at the volume that the gas takes up, the volume of the container, and the pressure of the gas. Let's see how our model can explain these observations.

GRAPHIC: Gas particles and change in pressure

NARRATOR (MUSIC under):
What happens to the pressure if the volume of the container is doubled, but the amount of gas particles is kept the same? As the volume of the container increases, the gas particles have more room to bounce around. They are now striking the wall only half as often as before. The pressure also drops back to half of what it was at the smaller volume of our gas.

MONTAGE: Geysers, hot springs, clouds, , kinetic particle model graphic, computer graphic model, chemists working in labs

NARRATOR (MUSIC and NAT SOUND under):
The kinetic particle model applies to any gas under standard conditions. However, in the real world, there are many different types of gases, and the particles of one gas are different from the particles of other gases. Yet, even though they are different, all groups of gas particles obey the general rules laid out in the kinetic particle model. This is true regardless of the type of gas particles. The kinetic particle model deals with the average behavior of large numbers of gas particles. It doesn't deal with the shape of single gas particles. But in other areas of chemistry, models of the actual shapes of single particles are very important. What you are looking at now is a model of a drug compound used to treat ulcers. These models have opened the door to an unseen world inside our bodies, a world where drug particles interact with cells on a submicroscopic invisible level. They have led to remarkable discoveries in the fields of biochemistry and drug research. (cont.)

NARRATOR cont:
Dr. David Pensak and a team at Du Pont are one of several groups creating computer models of particle structure. How are these models used in drug research?

INTERVIEW: Dr. David Pensak, The DuPont Company

SUPER: David Pensak

DR. DAVID PENSAK (SYNC/VO):
Computers are very nice tools to help us better understand how nature puts her building blocks together to create the substances which we encounter in our daily life.

Animated computer models

What you are looking at now is a computer graphics picture of DNA, the thread of life. What we're trying to understand, in any kind of a model,

INTERVIEW: Dr. David Pensak cont.

is exactly what's going on at the level whereby nature is doing whatever it is, is happening. We cannot get down

Animated computer models

small enough physically to see that. So what we have to do is try to simulate this. The problem is that these particles are so small (cont.)

INTERVIEW: Dr. David Pensak cont.

DR. DAVID PENSAK cont:
that, by and large, chemists who never really had the chance to create a mental picture of what they're like, so what we have to do is develop models to enable them to think about things that are too small for them to actually look at.

Animated computer models

NARRATOR:
The key and lock model is an example. Picture a drug as a key. The cells in our bodies each contain many different kinds of locks. One of these locks, if opened, could result in a desired effect. But to open the lock, the key must be an exact fit. Computer models help researchers imagine the properly shaped particle.

INTERVIEW: Dr. David Pensak cont.

DR. DAVID PENSAK (SYNC/VO):
The problem that we have is, yes, you have a key, and yes, it fits into a lock. We have to worry about how does the lock and the key actually find each other, because they're both swimming around inside the body. There has to be some process of recognition whereby the key knows, "This is the lock I want to interact with." And we call the process by which it approaches the lock, the docking problem. (cont.)

Animated computer models

DR. DAVID PENSAK cont:
We're trying to simulate it on the computer, very much the same as worrying about how a boat pulls up to a dock, how to recognize where the appropriate slip is. But what makes this different than the boat docking problem is that we have a very oddly shaped slip -- the hole in the lock, if you will -- and we have to make sure we put just the right key in there.

INTERVIEW: Dr. David Pensak cont.

Because if the key that we put in doesn't fit, you don't get the desired activity at all. And if we have a key that can fit into multiple locks, you begin to have a side effects problem.

MONTAGE: Bottles on assembly line, chemists working in labs, computer models, pill

NARRATOR (MUSIC under):
To create a new drug, researchers may need to synthesize hundreds of compounds and test each. It is expensive and time-consuming. Models streamline the process by identifying which particles have the highest potential for success. And because these models help researchers to see substances in new and different ways, they sometimes yield unexpected breakthroughs.

INTERVIEW: Dr. David Pensak cont.

DR. DAVID PENSAK (SYNC):
Let me tell a little story that's near and dear to my heart. For awhile we had two computer graphic systems side by side, and one of my people was working on developing a new class of weed killers, another one was working on a class of molecules which were involved in treating of cancer, truly a high priority item. As luck would have it, they were both working, and they both got telephone calls at the same moment. They went back to their laboratories. When they came back, they inadvertently got on each other's terminal. And about 15 seconds later the first one yelled out, "What are you working on my class of compounds for?" He said, "I'm not." He said, "Yes, this is my compound over here." What came out of this was there was a similarity between the weed killer and the anticancer drug that had never been recognized before. Because the way we had been used to drawing these structures on a sheet of paper, is in a stylized representation which is really almost artificial, and you would have never seen that similarity. But when you display them exactly as nature is really dealing with them, there was a striking similarity. (cont.)

DR. DAVID PENSAK cont:
We wound up submitting some of our weed killers to the National Cancer Institute for screening, and it turns up they've got really significant antitumor activity. But who in their right mind would have ever thought of even taking a weed killer and dreaming that it would have any kind of activity in dealing with cancer?

SUPER: MODELING THE UNSEEN

MONTAGE: Volcanos, clouds, chemists working in labs, computer models, program graphics, pills

NARRATOR (MUSIC under):
To review: We use models to understand events and processes that we cannot see or touch directly. To develop a model, the scientist starts with observations. These observations are used to form a mental representation, a model of the process being studied. Then the model must be tested. One important chemical model is the kinetic particle model of gases. It states that gases are composed of billions of submicroscopic particles in constant random motion. Models explain processes that vary from a very large scale to a very small scale, from the macro level to the micro level. (cont.)

NARRATOR cont:
They are used to understand the chemistry on the surface of distant planets, such as the massive sulfur volcanos on Io. And they are also used to predict the behavior of infinitesimally small drug particles inside our bodies. For the chemist, models are a crucial tool for understanding the unseen.

RH in an art gallery with chemical models

ROALD HOFFMANN (SYNC):
It turns out that I am actually very much a model builder. I want to tell you a little story about a piece of work. Actually, it was the work that won the Nobel prize for me and for Kenichi Fukui of Japan in 1981, and that involved building models. There is an important class of organic reactions in which a chain is converted into a ring. Now, that looks like a rather simple process. It turns out to be actually a very important one in the chemistry of Vitamin D. But when you look in detail at this process, all kinds of richnesses emerge. For instance, in the process of forming that ring, the two ends of the chain can rotate together, like this, so that the red lines are on one side of the ring. Or, alternatively, they can rotate in another way, and now you see that the red lines are on opposite sides of the ring. (cont.)

ROALD HOFFMANN cont:
Now, those are two different molecules, and the remarkable thing, and crucial for the chemistry of these molecules, is that one or the other of these rotations, not both, are followed, depending on the number of carbon atoms in the chain. Fukui and I were able to construct a model, using methods of physics, to explain this preference. That model, within a very short period, was tested by the experiments of many people around the world. I wish I could tell you that every model that I have built has been as successful as this one. Some have been, and some haven't. Enough have been right to keep me going.

Credits, Closing Montage, Closing Music

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